

L12 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:348009 CAPLUS Full-text

DN 140:356957

TI Preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation

IN Panten, Johannes; Fahlbusch, Karl-Georg; Werner, Matthias; Sillon, Pascal

PA Symrise GmbH & Co. KG, Germany

SO Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1413570	A1	20040428	EP 2003-22338	20031004
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	DE 10247966	A1	20040506	DE 2002-10247966	20021015
	US 2004127394	A1	20040701	US 2003-684726	20031014
	BR 2003004488	A	20040831	BR 2003-4488	20031014
	JP 2004137275	A2	20040513	JP 2003-354687	20031015

PRAI DE 2002-10247966 A 20021015

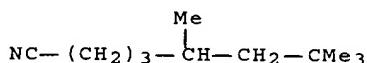
AB Fragrant 5,7,7-trimethyloctanenitrile, useful as a fragrance in bleaches, is prepared in high yield and selectivity via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde to give the mixed-isomer intermediate Z/E-5,7,7-Trimethyl-2(3)-octenenitriles which are then subjected to catalytic (e.g., Pd/C) hydrogenation.

IT 681449-57-0P

RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fragrant 5,7,7-trimethyloctanenitrile via the Knoevenagel condensation of cyanoacetic acid and isononylaldehyde followed by catalytic hydrogenation)

RN 681449-57-0 CAPLUS

CN Octanenitrile, 5,7,7-trimethyl- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:876124 CAPLUS Full-text
DN 138:187334
TI Exceptionally long ($\geq 2.9 \text{ \AA}$) CC bonding interactions in π -[TCNE]22- dimers: Two-electron four-center cation-mediated CC bonding interactions involving π^* electrons
AU Del Sesto, Rico E.; Miller, Joel S.; Lafuente, Pilar; Novoa, Juan J.
CS Department of Chemistry, University of Utah, Salt Lake City, UT,
84112-0850, USA
SO Chemistry--A European Journal (2002), 8(21), 4894-4908
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Three groups of singlet ground state [TCNE]22- (TCNE = tetracyanoethylene) dimers with characteristic intradimer CC sepns. (r) and dihedral angles (d) [i.e., group St (r .apprx. 1.6 \AA ; d = 180°), Lt (r .apprx. 3.5 \AA ; d = 180°), and Lc (r .apprx. 2.9 \AA ; d = .apprx. 0°); notation: S/L: short/long bond length; subscript t/c: trans/cis, resp.] are exptl. characterized. The St group is comprised of σ -dimers of [TCNE]•- and octacyanobutanediide, [C₄(CN)₈]2-, which have a typical, albeit long, sp³-sp³ σ bond (r .apprx. 1.6 \AA) between each [TCNE]•- moiety and characteristic vCN, vCC, and δ CCN IR absorptions. The L groups are structurally characterized as π -dimers of [TCNE]•- that are either eclipsed with r .apprx. 2.9 \AA (Lc) and the nitriles bend away from the nominal TCNE plane away from the center of the dimer by 5.0° (.apprx.sp2.17) or are noneclipsed with r .apprx. 3.5 \AA (Lt) and the nitriles bend toward the center of the dimer by 1.9° (.apprx.sp2.06). Ab initio computations on isolated dimers were used to study the formation and stability of these exceptionally long CC ($\geq 2.9 \text{ \AA}$) bonding interactions as well as the process of π -[TCNE]22- dimer formation for the Lc and Lt groups. The results of these computational studies show that the ground-state potential curve is that of a closed-shell/open-shell singlet, depending on the distance. The short St group (r .apprx. 1.6 \AA) of dimers in this surface are true min.-energy structures; however, the Lt and Lc groups are unstable, although two different nonphys. min. are found when imposing a double occupancy of the orbitals. These min. are metastable relative to dissociation into the isolated [TCNE]•- units. Consequently, the existence of dimer dianions in crystals is due to cation ... [TCNE]- interactions, which provide the electrostatic stabilization necessary to overcome the intradimer electrostatic repulsion. This cation-mediated π^* - π^* [TCNE]- ... [TCNE]- interaction complies with Pauling's definition of a chemical bond. This bonding interaction involves the π^* orbitals of each fragment, and arise from the overlap of the b_{2g} SOMO on each of the two [TCNE]•-s to form a filled b_{2u} [TCNE]22- orbital. Although a π dimer typically forms, if the fragments are close enough a σ dimer can form. Due to the presence of cation-mediated intradimer CC bonding interactions the Lc group of π -[TCNE]22- dimers exhibits exptl. observable vCN IR absorptions at 2191 ± 2 (m), 2173 ± 3 (s), and 2162 ± 3 cm⁻¹ (s) and vCC at 1364 ± 3 cm⁻¹ (s) as well as a new UV-Vis feature in the range of 15000 to 18200 cm⁻¹ (549 to 667 nm) and averaging 16825 ± 1180 cm⁻¹ (594 nm) assigned to the predicted new intradimer 1A_{1g} → 1B_{1u} transition and is purple on reflected light. Upon cooling to 77 K in 2-methyltetrahydrofuran, this

new band occurs at 18940 cm⁻¹ (528 nm) for {[Et₄N]⁺}₂[TCNE]22-, and the yellow solution turns deep red. Group Lt is characterized by νCN absorptions at 2215 ± 2, 2197 ± 3, and 2180 ± 4 cm⁻¹ and νCC at 1209 ± 9 cm⁻¹ (w), while group ST has νCN bands at 2215 ± 4, 2157 ± 3, and 2107 ± 4 cm⁻¹ and νCC at 1385 ± 1 cm⁻¹ (vs).

IT 210233-00-4

RL: PRP (Properties)

(exceptionally long CC bonding interactions in π-[TCNE]22- dimers with two-electron four-center cation-mediated CC bonding interactions involving π* electrons)

RN 210233-00-4 CAPLUS

CN Iron(2+), bis(acetonitrile)-, salt with 1,1,2,2,3,3,4,4- butaneoctacarbonitrile, compd. with acetonitrile (1:1:1) (9CI) (CA

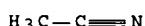
INDEX

NAME)

CM 1

CRN 75-05-8

CMF C2 H3 N



CM 2

CRN 210232-99-8

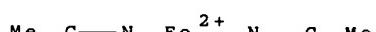
CMF C12 N8 . C4 H6 Fe N2

CM 3

CRN 210232-98-7

CMF C4 H6 Fe N2

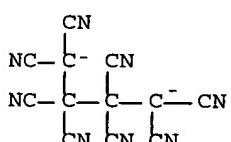
CCI CCS



CM 4

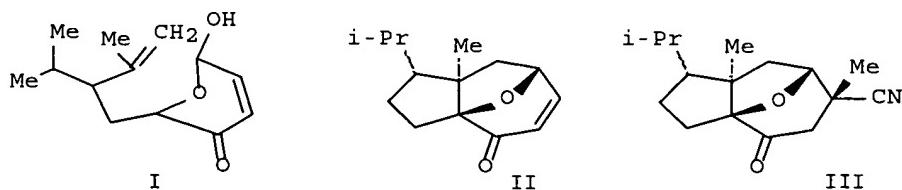
CRN 210232-94-3

CMF C12 N8



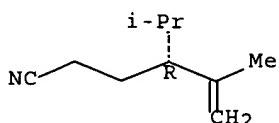
RE.CNT 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:498880 CAPLUS Full-text
 DN 135:304028
 TI Stereoselective synthesis of the bicyclo[5.3.0]decane portion of the diterpene antibiotic guanacastepene using a pyrylium-ylide [5+2] cycloaddition reaction
 AU Magnus, P.; Waring, M. J.; Ollivier, C.; Lynch, V.
 CS Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712, USA
 SO Tetrahedron Letters (2001), 42(30), 4947-4950
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 OS CASREACT 135:304028
 GI

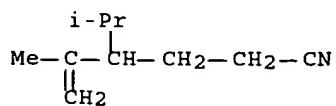


AB Treatment of I with Ac₂O/Et₃N resulted in [5+2] cyclization to give II, which was further elaborated into III, thus establishing the required stereochem. in the top-half of guanacastepene.
 IT 365978-34-3P 365978-53-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (stereoselective synthesis of bicyclo[5.3.0]decane portion of diterpene
 antibiotic guanacastepene using a pyrylium-ylide [5+2] cycloaddn. reaction)
 RN 365978-34-3 CAPLUS
 CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 365978-53-6 CAPLUS
 CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



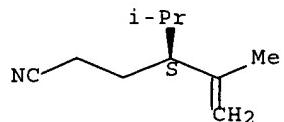
IT 365978-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of bicyclo[5.3.0]decane portion of
diterpene
antibiotic guanacastepene using a pyrylium-ylide [5+2] cycloaddn.
reaction)

RN 365978-51-4 CAPLUS

CN 5-Hexenenitrile, 5-methyl-4-(1-methylethyl)-, (4S)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).



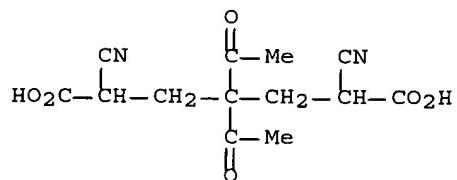
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:148131 CAPLUS Full-text
 DN 132:278725
 TI Self-catalytic Michael reaction. An efficient route to 2-cyanoalkanoic acids
 AU Krawczyk, Henryk
 CS Institute of Organic Chemistry, Technical University (Politechnika), Lodz,
 90924, Pol.
 SO Synthetic Communications (2000), 30(4), 657-664
 CODEN: SYNCV; ISSN: 0039-7911
 PB Marcel Dekker, Inc.
 DT Journal
 LA English
 OS CASREACT 132:278725
 AB The self-catalytic Michael reaction of several 1,3-dicarbonyl compds. with dicyclohexylammonium 2-cyanoacrylate proceeded highly efficiently at room temperature to give the corresponding 1,4-adducts.
 IT 263703-46-4p
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (self-catalytic Michael reaction in preparation of 2-cyanoalkanoic acids)
 RN 263703-46-4 CAPLUS
 CN Heptanedioic acid, 4,4-diacetyl-2,6-dicyano-, compd. with N-cyclohexylcyclohexanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 263703-45-3

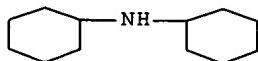
CMF C13 H14 N2 O6



CM 2

CRN 101-83-7

CMF C12 H23 N

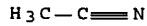


RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:433463 CAPLUS Full-text
DN 129:130514
TI Isolation and structural determination of octacyanobutanediide,
[C₄(CN)₈]₂-; precursors to M(TCNE)_x magnets
AU Zhang, Jie; Del Sesto, Rico E.; Gordon, Douglas C.; Miller, Joel S.;
Zhang, Jie; Liable-Sands, Louise M.; Rheingold, Arnold L.; Burkhardt,
Brian
M.
CS Department of Chemistry, University of Utah, Salt Lake City, UT,
84112-0850, USA
SO Chemical Communications (Cambridge) (1998), (13), 1385-1386
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB The reaction of MI₂·xMeCN (M = Mn, Fe) and TCNE (tetracyanoethylene)
leads to unprecedented [C₄(CN)₈]₂- μ₄-metal complexes which were
crystallog. characterized and are precursors to M(TCNE)_x·yS magnets.
IT 210233-00-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation, crystal structure of polymeric μ₄-octacyanobutanediide
complex, and thermal decomposition to give metal TCNE magnet)
RN 210233-00-4 CAPLUS
CN Iron(2+), bis(acetonitrile)-, salt with 1,1,2,2,3,3,4,4-
butaneoctacarbonitrile, compd. with acetonitrile (1:1:1) (9CI) (CA
INDEX
NAME)

CM 1

CRN 75-05-8
CMF C₂ H₃ N

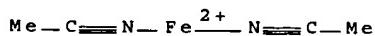


CM 2

CRN 210232-99-8
CMF C₁₂ N₈ . C₄ H₆ Fe N₂

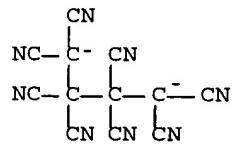
CM 3

CRN 210232-98-7
CMF C₄ H₆ Fe N₂
CCI CCS



CM 4

CRN 210232-94-3
CMF C12 N8



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:604511 CAPLUS Full-text

DN 121:204511

TI Facile preparation of conjugated dienes from allylic alcohols

AU Kitahara, Takeshi; Matsuoka, Tatsuji; Kiyota, Hiromasa; Warita, Yasuhiro;

Kurata, Hitoshi; Horiguchi, Akira; Mori, Kenji

CS Department of Agricultural Chemistry, University of Tokyo, Tokyo, 113, Japan

SO Synthesis (1994), (7), 692-4

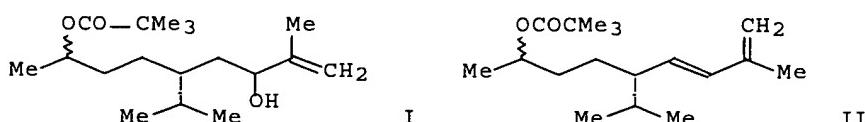
CODEN: SYNTBF; ISSN: 0039-7881

DT Journal

LA English

OS CASREACT 121:204511

GI



AB An efficient two-step procedure to prepare conjugated dienes from allylic alcs. is developed without the formation of regioisomers and rearranged products. Thus, to a solution of I and dry Et₃N in dry CH₂Cl₂ was added dropwise methanesulfonyl chloride; after workup, the crude mesylate was dissolved in diisopropylethylamine (Hunig's base) and dry HMPA and heated at 160° for 20 min. to give (2RS,5R)-8-methyl-5-(1-methylethyl)-6,8- nonadien-2-yl pivalate (II) in 64% yield.

IT 157905-12-9P

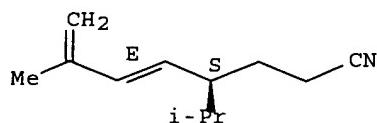
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 157905-12-9 CAPLUS

CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, [S-(E)]- (9CI) (CA INDEX NAME)

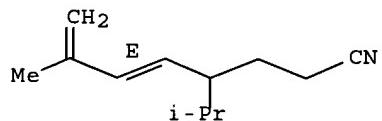
Absolute stereochemistry.

Double bond geometry as shown.



L12 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:134846 CAPLUS Full-text
DN 120:134846
TI A new synthesis of solanone
AU Park, Oee Sook; Kim, Hong Jin; Chae, Woo Ki; Lee, Woo Young
CS Dep. Chem., Chungbuk Natl. Univ., Chungbuk, 306-763, S. Korea
SO Bulletin of the Korean Chemical Society (1993), 14(5), 639-41
CODEN: BKCSDE; ISSN: 0253-2964
DT Journal
LA English
OS CASREACT 120:134846
AB A new synthesis of solanone, (E)-MeCOCH₂CH₂CH(CHMe₂)CH:CHCMe:CH₂, suitable for use in the perfume industry, is described. Et isovalerate or di-Me malonate are the readily available starting materials.
IT 51513-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in preparation of solanone from isovalerate or malonate)
RN 51513-11-2 CAPLUS
CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

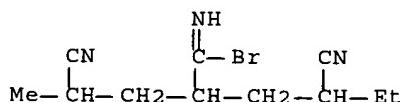


L12 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1994:129084 CAPLUS Full-text
 DN 120:129084
 TI Polyacrylonitrile modified with hydrogen halide for immobilization of biological substances
 IN Howard, Edward G., Jr.; Shannon, Patrick T.
 PA du Pont de Nemours, E. I., and Co., USA
 SO U.S., 7 pp. Cont. of U.S. Ser. No. 641,991, abandoned.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5262317	A	19931116	US 1992-939567	19920903
PRAI US 1988-275189	B1	19881123		
US 1991-641991	B1	19910116		

AB Polyacrylonitrile is chemical modified with HX (X = Cl, Br, I, CF₃SO₃) to produce a polymer with readily replaceable X groups. The modified polyacrylonitrile is useful as an immobilization substrate for, e.g., proteins and in affinity chromatog. Preparation of the halo-modified polyacrylonitriles is included. Immobilization of an anti-apoprotein B monoclonal antibody and of Staphylococcus aureus-derived protein A is described.
 IT 153087-08-2 153087-12-8 153087-16-2
 153087-20-8
 RL: ANST (Analytical study)
 (for biol. material immobilization)
 RN 153087-08-2 CAPLUS
 CN Hexanimidoyl bromide, 4-cyano-2-(2-cyanopropyl)-, polymer with 2-propenenitrile (9CI) (CA INDEX NAME)

CM 1
 CRN 153087-07-1
 CMF C11 H16 Br N3



CM 2

CRN 107-13-1
 CMF C3 H3 N

H₂C=CH-C≡N

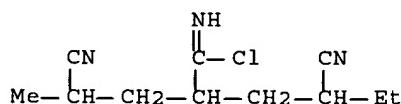
RN 153087-12-8 CAPLUS

CN Hexanimidoyl chloride, 4-cyano-2-(2-cyanopropyl)-, polymer with
2-propenenitrile (9CI) (CA INDEX NAME)

CM 1

CRN 153087-11-7

CMF C11 H16 Cl N3



CM 2

CRN 107-13-1

CMF C3 H3 N



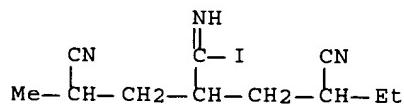
RN 153087-16-2 CAPLUS

CN Hexanimidoyl iodide, 4-cyano-2-(2-cyanopropyl)-, polymer with
2-propenenitrile (9CI) (CA INDEX NAME)

CM 1

CRN 153087-15-1

CMF C11 H16 I N3



CM 2

CRN 107-13-1

CMF C3 H3 N

H₂C≡CH—C≡N

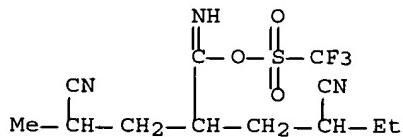
RN 153087-20-8 CAPLUS

CN Hexanimidic acid, 4-cyano-2-(2-cyanopropyl)-, anhydride with trifluoromethanesulfonic acid, polymer with 2-propenenitrile (9CI) (CA INDEX NAME)

CM 1

CRN 153087-19-5

CMF C12 H16 F3 N3 O3 S



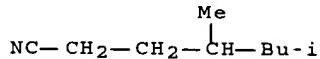
CM 2

CRN 107-13-1

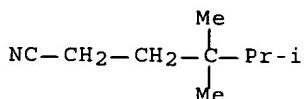
CMF C3 H3 N

H₂C≡CH—C≡N

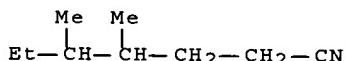
L12 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:160132 CAPLUS Full-text
DN 116:160132
TI Thermochemical parameters of nitriles in the ideal gas state
AU Bures, Michal; Cerny, Cestmir; Holub, Robert
CS Vys. Sk. Chemickotechnol., Prague, Czech.
SO Chemicky Prumysl (1990), 40(11-12), 589-95
CODEN: CHPUA4; ISSN: 0009-2789
DT Journal
LA Czech
AB The functional group contribution approach was used to derive the parameters of the equations for the calcn. of the heat capacities and free energy functions of alkyl nitriles (C5-C9). The values of these parameters for compds. are tabulated.
IT 78695-45-1, 4,6-Dimethylheptanonitrile 99064-65-0,
4,4,5-Trimethylhexanonitrile 138807-85-9, 4,5-
Dimethylheptanonitrile 138807-91-7, 5,6-Dimethylheptanonitrile
138807-97-3, 3,4,5-Trimethylhexanonitrile 138808-02-3,
2,4,5-Trimethylhexanonitrile 138808-04-5, 4,5,5-
Trimethylhexanonitrile 138808-14-7, 4-Ethyl-5-
methylhexanonitrile 138808-42-1, 4,5-Dimethylhexanonitrile
RL: PRP (Properties)
(free energy function and heat capacity equations for, parameters for,
in ideal gas state)
RN 78695-45-1 CAPLUS
CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)



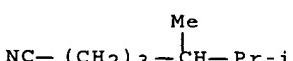
RN 99064-65-0 CAPLUS
CN Hexanenitrile, 4,4,5-trimethyl- (9CI) (CA INDEX NAME)



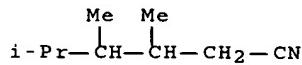
RN 138807-85-9 CAPLUS
CN Heptanenitrile, 4,5-dimethyl- (9CI) (CA INDEX NAME)



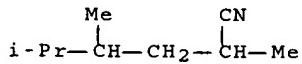
RN 138807-91-7 CAPLUS
CN Heptanenitrile, 5,6-dimethyl- (9CI) (CA INDEX NAME)



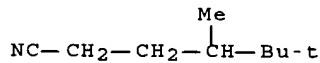
RN 138807-97-3 CAPLUS
CN Hexanenitrile, 3,4,5-trimethyl- (9CI) (CA INDEX NAME)



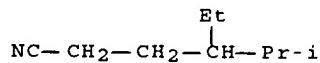
RN 138808-02-3 CAPLUS
CN Hexanenitrile, 2,4,5-trimethyl- (9CI) (CA INDEX NAME)



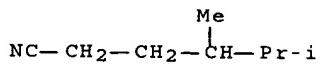
RN 138808-04-5 CAPLUS
CN Hexanenitrile, 4,5,5-trimethyl- (9CI) (CA INDEX NAME)



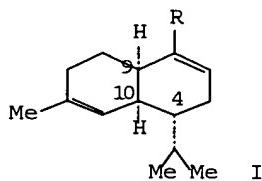
RN 138808-14-7 CAPLUS
CN Hexanenitrile, 4-ethyl-5-methyl- (9CI) (CA INDEX NAME)



RN 138808-42-1 CAPLUS
CN Hexanenitrile, 4,5-dimethyl- (9CI) (CA INDEX NAME)

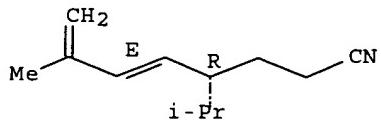


L12 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1987:5248 CAPLUS Full-text
 DN 106:5248
 TI Synthetic microbial chemistry. XII. Synthesis of both enantiomers of sclerosporin and sclerosporal, sporogenic substances of Sclerotinia fructicola
 AU Kitahara, Takeshi; Kurata, Hitoshi; Matsuoka, Tatsuji; Mori, Kenji
 CS Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan
 SO Tetrahedron (1985), 41(23), 5475-85
 CODEN: TETRAB; ISSN: 0040-4020
 DT Journal
 LA English
 OS CASREACT 106:5248
 GI

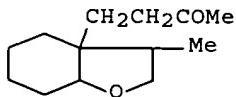


AB Both enantiomers of sclerosporin and sclerosporal were synthesized from (-)-carvone. (4R,9R,10S)-(+)-Sclerosporin (I, R = CO₂H) and (4R,9R,10S)-(-)-sclerosporal (I, R = CHO) were identified as the natural enantiomers by a comparison of their CD spectra. An intramol. Diels-Alder route proved to be an efficient method of preparing sufficient amts. of I for future biol. study.
 IT 105661-26-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for sclerosporin)
 RN 105661-26-5 CAPLUS
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, [R-(E)]- (9CI) (CA INDEX NAME)

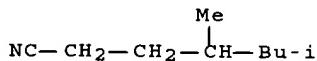
Absolute stereochemistry.
 Double bond geometry as shown.



L12 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1986:405818 CAPLUS Full-text
DN 105:5818
TI Denitrohydrogenation of aliphatic nitro compounds and a new use of aliphatic nitro compounds as radical precursors
AU Ono, Noboru; Miyake, Hideyoshi; Kamimura, Akio; Hamamoto, Isami; Tamura, Rui; Kaji, Aritsune
CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
SO Tetrahedron (1985), 41(19), 4013-23
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 105:5818
GI



AB Denitrohydrogenation of RR₁R₂CNO₂ (R-R₂ = alkyl, aryl) by Bu₃SnH in C₆H₆ in the presence of AIBN gave RR₁R₂CH. Compds. activated by CN, COR, or CO₂R groups, e.g., PhCOCMe₂NO₂, were readily denitrohydrogenated. Presence of radical leaving groups gave elimination reactions in some cases; thus, treating PhCH(NO₂)CH(SPh)Ph with Bu₃SnH gave only E-PhCH:CHPh, with no product resulting from denitrohydrogenation. The radical intermediates generated by denitration were also used in C-C: reforming reactions, e.g., cyclization. Thus, treating (allyloxy)nitrocyclohexane with Bu₃SnH gave a high yield of the furan derivative I. Also used as the C-C bond-forming reaction was the intermol. addition of radicals to alkenes.
IT 78695-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by denitrohydrogenation of nitroalkane)
RN 78695-45-1 CAPLUS
CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)



L12 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:504806 CAPLUS Full-text

DN 103:104806

TI The Prins-type reactions of mono- and 1,1-disubstituted alkenes with trichloroacetonitrile in the presence of boron trichloride

AU Hamana, Hiroshi; Sugasawa, Tsutomu

CS Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan

SO Chemistry Letters (1985), (5), 571-4

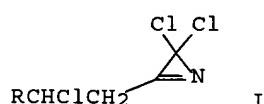
CODEN: CMLTAG; ISSN: 0366-7022

DT Journal

LA English

OS CASREACT 103:104806

GI



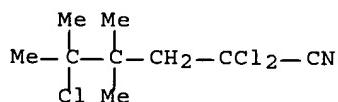
AB BC₁₃ catalyzed the Prins-type reaction of alkenes RCH:CH₂ (R = hexyl, Bu, Me₂CHCH₂, EtCHMe, Me₃C, PhCH₂) with Cl₃CCN to give dichloroazirines I in high yields. Further exposure of I to BC₁₃ at room temperature afforded RCHClCH₂CCl₂CN. The Prins-type acylations of R₁R₂C:CH₂ [R₁R₂ = (CH₂)₅, (CH₂)₃; R₁ = R₂ = Et; R₁ = CMe₃, CHMe₂, R₂ = Me], limonene, and camphene with Cl₃CCN gave R₁R₂CClCH₂COCl₃ and R₁R₂C:CHCOCCl₃.

IT 97963-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 97963-01-4 CAPLUS

CN Hexanenitrile, 2,2,5-trichloro-4,4,5-trimethyl- (9CI) (CA INDEX NAME)



L12 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1981:496925 CAPLUS Full-text

DN 95:96925

TI A new synthetic method: direct replacement of the nitro group by hydrogen

or deuterium

AU Ono, Noboru; Miyake, Hideyoshi; Tamura, Rui; Kaji, Aritsune

CS Dep. Chem., Kyoto Univ., Kyoto, 606, Japan

SO Tetrahedron Letters (1981), 22(18), 1705-8

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 95:96925

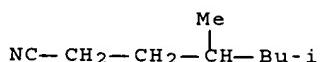
AB Bu₃SnR (R = H, D) denitrate tertiary or secondary aliphatic and aryl nitro compds. to give the corresponding alkanes or deuteroalkanes. Thus, treatment of Me₃CCH₂CMe₂NO₂ with Bu₃SnH in refluxing C₆H₆ in the presence of AIBN for 2 h gave 75 % Me₃CCH₂CHMe₂. Similarly, treatment of 4-NCC₆H₄CMe₂NO₂ with Bu₃SnD in C₆H₆-AIBN for 1.5 h gave 85% 4-NCC₆H₄CDMe₂.

IT 78695-45-1P

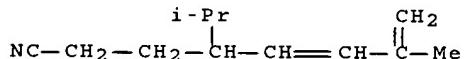
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by denitration reaction)

RN 78695-45-1 CAPLUS

CN Heptanenitrile, 4,6-dimethyl- (9CI) (CA INDEX NAME)

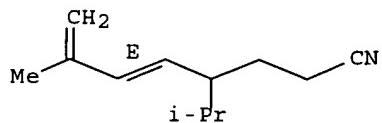


L12 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1979:439653 CAPLUS Full-text
 DN 91:39653
 TI Synthesis of methyl 4-isopropyl-7-methyl-5,7-octadienoate
 AU Watanabe, Shoji; Fujita, Tsutomu; Suga, Kyoichi; Inaba, Teruhiko;
 Tsuruta,
 Haruki
 CS Fac. Eng., Chiba Univ., Chiba, Japan
 SO Yukagaku (1979), 28(2), 115-16
 CODEN: YKGKAM; ISSN: 0513-398X
 DT Journal
 LA Japanese
 OS CASREACT 91:39653
 AB Analogs of solanone were prepared Condensation of Me₂CHCH₂CHO piperidine enamine with CH₂:CHCO₂Me and CH₂:CHCN gave RCH₂CH₂CH(CHMe₂)CHO [R = CO₂Me (I) and CN (II); resp.]. Wittig reaction of I with CH₂:CMeCH:PPh₃ in THF gave H₂C:CMeCH:CHCH(CHMe₂)CH₂CH₂R₁ (III; R₁ = CO₂Me). Similarly II gave III (R₁ = CN), hydrolysis of which under basic condition gave cis- and trans-Me₂C:CHCH:C(CHMe₂)CH₂CH₂CO₂Me.
 IT 70687-52-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT
 (Reactant or reagent)
 (preparation and hydrolysis of)
 RN 70687-52-4 CAPLUS
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

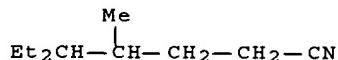


L12 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1978:538029 CAPLUS Full-text
 DN 89:138029
 TI Nuclear magnetic resonance study of metal complexes. 2. Conformations
 of
 1,2-diamine chelate rings with C-phenyl group(s) in cobalt(III) and
 platinum(II) complexes
 AU Yano, S.; Tukada, T.; Saburi, M.; Yoshikawa, S.
 CS Fac. Eng., Univ. Tokyo, Tokyo, Japan
 SO Inorganic Chemistry (1978), 17(9), 2520-6
 CODEN: INOCAJ; ISSN: 0020-1669
 DT Journal
 LA English
 AB The proton NMR spectra of $[\text{Co}(\text{CN})_4(\text{R-phenyl})]$ ($\text{R- phenyl} = \text{R-phenylethylenediamine}$), $[\text{Pt}(\text{NH}_3)_2(\text{pn-d1})]^{2+}$ ($\text{pn-d1} = 2\text{-deuterio-1,2-aminopropane}$), $[\text{Pt}(\text{S-pn-d2})_2]^{2+}$ ($\text{S-pn-d2} = (2\text{S})\text{-1,1-dideuterio-1,2,-aminopropane}$), $[\text{Pt}(\text{S,S-bn})_2]^{2+}$ ($\text{S,S-n} = (2\text{S},3\text{S})\text{-2,3-butanediamine}$)
 $[\text{Pt}(\text{en})((\text{-})\text{D-stein})]^{2+}$ (($\text{-1})\text{D-stien} = \text{silbenediamine}$) were measured for the diamine chelates with C-Ph group(s) a Karplus-like dihedral angle dependence for the $J_{\text{Pt-N-C-C}}$, where C+ is a Ph atom which attaches on the membered-C atom, was observed. These $J_{\text{Pt-N-C-CH3}}$ values were very similar to those for the $J_{\text{Pt-N-C-CH3}}$ in the diamine chelates with C-Me group(s).
 IT 51513-11-2
 RL: PRP (Properties)
 (NMR and conformation of)
 RN 51513-11-2 CAPLUS
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX
 NAME)

Double bond geometry as shown.

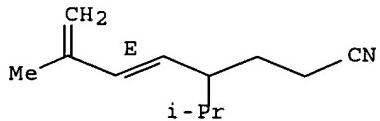


L12 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:433624 CAPLUS Full-text
DN 85:33624
TI Functionalization of unsaturated polymers. Action of chloroacetonitrile in basic media on polyalkadiene organoborane derivatives
AU Pinazzi, C. P.; Vassort, J.; Noireaux, P.; Reyx, D.
CS Lab. Chim. Org. Macromol., Cent. Univ., Le Mans, Fr.
SO European Polymer Journal (1976), 12(2), 83-6
CODEN: EUPJAG; ISSN: 0014-3057
DT Journal
LA French
AB Poly(1,2-butadiene), poly(1,4-butadiene) [9003-17-2], poly(3,4-isoprene) [9003-31-0], and poly(1,4-isoprene) and models of their structural repeating units, i.e. 3-ethylpentene [4038-04-4], 4-octene [592-99-4], 3-ethyl-2-methylpentene [19780-66-6], and 4-methyl-4-octene [38304-63-1] were treated with 9-borabicyclononane [25301-61-5] and then with K tert-butyloxide and ClCH₂CN. The monomers gave 65-84% yields of products with the cyanomethyl groups attached to the least substituted C and cyanomethylated polymer yields were 60-82% depending on microstructure.
IT 59333-88-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59333-88-9 CAPLUS
CN Heptanenitrile, 5-ethyl-4-methyl- (9CI) (CA INDEX NAME)

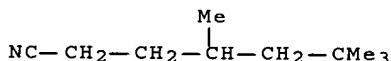


L12 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1974:45798 CAPLUS Full-text
 DN 80:45798
 TI Tobacco chemistry. 20. Structures and syntheses of three new tobacco constituents of probable isoprenoid origin
 AU Aasen, Arne J.; Hlubucek, Joseph R.; Almqvist, Sven; Kimland, Bjarne; Enzell, Curt R.
 CS Res. Dep., Swed. Tob. Co., Stockholm, Swed.
 SO Acta Chemica Scandinavica (1947-1973) (1973), 27(7), 2405-10
 CODEN: ACSAA4; ISSN: 0001-5393
 DT Journal
 LA English
 AB The structures of 3 new tobacco isolates, 5ζ -isopropyl-3E-hepten-2-one, 3ζ -hydroxy- 3ζ -methyl- 6ζ -isopropyl-4E-octenoic acid, and 2,10-dimethyl- 7ζ -isopropyl-8E-10-undecadien-4-one have been elucidated on the basis of their spectral data and subsequently confirmed by total syntheses. The possible isoprenoid origin of these compds. is discussed.
 IT 51513-11-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with isobutylmagnesium bromide)
 RN 51513-11-2 CAPLUS
 CN 5,7-Octadienenitrile, 7-methyl-4-(1-methylethyl)-, (E)- (9CI) (CA INDEX NAME)

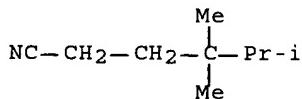
Double bond geometry as shown.



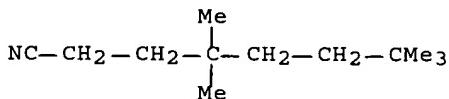
L12 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1965:438851 CAPLUS Full-text
DN 63:38851
OREF 63:6913e-h
TI Reduction of aromatic and branched-chain aliphatic nitriles by SnCl₂
(Stephen aldehyde synthesis)
AU Pyryalova, P. S.; Zil'berman, E. N.
SO Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya
Tekhnologiya (1965), 8(1), 82-7
CODEN: IVUKAR; ISSN: 0579-2991
DT Journal
LA Russian
AB The Stephen aldehyde synthesis, reduction of nitriles by treatment with anhydrous SnCl₂ dissolved in Et₂O saturated with HCl and subsequent hydrolysis of the aldimines formed, was investigated for determination of optimum reaction conditions. Using PhCN, the following factors were found to influence the yield of BzH: (1) the Et₂O solution of PhCN should be saturated with HCl gas and the resulting mixture kept 3-4 hrs.; (2) the reaction temperature should be 20° (89% yield BzH) rather than 0° (85%); (3) the molar ratio RCN-SnCl₂ of 1:2 (100%) instead of 1:1.1 (74%); (4) a stream of HCl gas should be conducted through the combined solns. of RCN and SnCl₂ until the solution is homogeneous; precipitation of the aldimine hexachlorostannates then began after some time. After 3 days standing it was filtered, hydrolyzed with warm H₂O and the aldehyde steam-distilled. The following p-substituted benzaldehydes were obtained in this way in excellent yields (substituent given): Me, MeO, Cl, and Br. In p-NO₂- and m-O₂NC₆H₄CN at 0° only the NO₂ group was reduced. Increasing the RCN-SnCl₂ ratio to 1:6 did not affect p-O₂NC₆H₄CN; however it lead to 29% m-O₂NC₆H₄CHO and 61% m-H₂NC₆H₄CN. Reduction of both functional groups has been achieved in neither m- nor p-nitrobenzonitrile. Generally, electron donating substituents increased the nucleophilic properties of the nitrile group and facilitated aldimine formation, and conversely. In contrast to straight-chain aliphatic nitriles, which give bisamides, branched-chain aliphatic nitriles with more than 7 C atoms (RCN-SnCl₂ = 1:1.1, after 8 days standing) are converted readily, but with low yields into the corresponding aldehydes, as was shown with 3-ethylenanthonitrile, 2-methylcapronitrile and 4,6,6-trimethylenanthonitrile.
IT 2570-95-8, Heptanenitrile, 4,6,6-trimethyl-
(reduction with SnCl₂)
RN 2570-95-8 CAPLUS
CN Heptanenitrile, 4,6,6-trimethyl- (7CI, 9CI) (CA INDEX NAME)



L12 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1961:17973 CAPLUS Full-text
 DN 55:17973
 OREF 55:3606b-d
 TI 5-Neopentyl-5-allylbarbituric acid and related compounds. I. Preparation
 of β -tert-alkylpropionic acids and derivatives
 AU Brandstrom, Arne
 CS Pharmacia Ltd., Uppsala, Swed.
 SO Acta Chemica Scandinavica (1959), 13, 613-15
 CODEN: ACHSE7; ISSN: 0904-213X
 DT Journal
 LA English
 AB cf. ibid. 10, 1197(1956). 5-Neopentyl-5-allylbarbituric acid, a good
 sedative, was synthesized from $\text{ClCH}_2\text{CH}_2\text{CMe}_3$, readily converted into 94%
 $\text{Me}_3\text{CCH}_2\text{CH}_2\text{CN}$ (I), b5 57-9°; 93% $\text{EtCMe}_2\text{CH}_2\text{CH}_2\text{CN}$, b. 76-80, 91%
 $\text{Me}_2\text{CHCMe}_2\text{CH}_2\text{CH}_2\text{CN}$, b8 88-9°, and 80% $\text{Me}_3\text{CCH}_2\text{CH}_2\text{CMe}_2\text{CH}_2\text{CH}_2\text{CN}$, b8 107-10°,
 were similarly prepared. The cyanides were hydrolyzed to 77% $\text{Me}_3\text{CCH}_2\text{CH}_2\text{CO}_2\text{H}$ (II), b8 104-5°, 46% $\text{EtCMe}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$, b10 112-20°, and 50%
 $\text{Me}_2\text{CHCMe}_2\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$, b8 129-35°. II was also prepared by hydrogenating
 β -tert-butylacrylic acid over Pd-C; the Et ester of II, b8 60-2°, was
 prepared (86% yield) by refluxing II 8 hrs. with EtOH.
 IT 99064-65-0, Hexanenitrile, 4,4,5-trimethyl- 100247-00-5,
 Octanenitrile, 4,4,7,7-tetramethyl-
 (preparation of)
 RN 99064-65-0 CAPLUS
 CN Hexanenitrile, 4,4,5-trimethyl- (9CI) (CA INDEX NAME)



RN 100247-00-5 CAPLUS
 CN Octanenitrile, 4,4,7,7-tetramethyl- (6CI) (CA INDEX NAME)



L12 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1952:5236 CAPLUS Full-text

DN 46:5236

OREF 46:879b-i

TI Synthesis and reactions of branched-chain hydrocarbons. I. Hydrocarbons with the 3,5,5-trimethylhexyl groups

AU Gutman, E. M.; Hickinbottom, W. J.

CS Queen Mary Coll., London

SO Journal of the Chemical Society, Abstracts (1951) 2064-7

CODEN: JCSAAZ; ISSN: 0590-9791

DT Journal

LA Unavailable

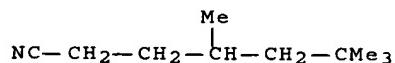
AB This series considers the reactions and properties of paraffins with a regular pattern of quaternary C atoms; this first paper deals with the possibilities and limitations of alkylmagnesium halides having quaternary C atoms for such syntheses. $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{OH}$ (I) (144 g.) in 79 g. $\text{C}_5\text{H}_5\text{N}$, treated gradually (with stirring and cooling) with 125 g. SOCl_2 , stirred an addnl. 20 min., gradually heated to 110° , and kept at that temperature 2-4 hrs. (cessation of evolution of SO_2), gives 91% $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{Cl}$ (II), $b_{17} 70^\circ$, $n_{D25} 1.4304$. II is hydrolyzed very slowly by aqueous alkali; it reacts only sluggishly in ether with Mg. The Grignard reagent (III) can be prepared in 78% yield after starting the reaction with MeI . Oxidation of III gives 67% I. I (19.8 g.), 60 g. 48% HBr, and 15.6 g. concentrated H_2SO_4 , refluxed 6 hrs., give 70% 1-bromo analog of II, $b_{12} 75^\circ$, $n_{D20} 1.4527$. III from 65 g. II, 9.8 g. Mg, and 150 ml. ether, added to 14.4 g. AcOEt and refluxed, gives 78% 2,2,4,7,10,12,12-heptamethyl-7-tridecanol (IV), $b_{9.5} 120^\circ$, $n_{D20} 1.4512$; IV and a little iodine, heated until H_2O formation ceases (0.5 hr.) and the residue refluxed 3 hrs. over Na, give a product composed largely of 2,2,4,7,10,12,12-heptamethyl-6-tridecene (V) [with some $(\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2)_2\text{C:CH}_2$], $b_{0.55} 101-3^\circ$, $n_{D20} 1.4389-98$. With O_3 , 22 g. V yields HCHO , 10.3 g. 5,7,7-trimethyl-2-octanone (VI), $b_{28} 103^\circ$, $n_{D20} 1.4309$ (semicarbazone, m. $147.5-8.5^\circ$; 2,4-dinitrophenylhydrazone, m. 80°), 0.6 g. $b_{1.3} 120-34^\circ$, and 4.6 g. $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CO}_2\text{H}$ (VII) (S-benzylthiuronium salt, m. 154°). Hydrogenation of V in EtOH over Raney Ni at $150^\circ/39$ atmospheric gives 79% 2,2,4,7,10,12,12-heptamethyltridecane, $b_{0.5} 112^\circ$, $n_{D20} 1.4437$, $d_{1919} 0.7901$. $\text{Me}_3\text{CCH}_2\text{CHMeCH}_2\text{CH}_2\text{CN}$ (5.3 g.) and MeMgI give 1.6 g. VI. III from 19.5 g. II in ether, refluxed 3 hrs. with CdCl_2 , the ether replaced by 70 ml. C_6H_6 , and treated with 7.6 g. AlCl_3 in 20 ml. C_6H_6 , gives 6.1 g. VI. II (97.5 g.) and 78 g. KCN in 75 ml. H_2O and 170 ml. EtOH , refluxed 72 hrs., give 59.5 g. 1-cyano-3,5,5-trimethylhexane (VII), $b_{11} 97-8^\circ$, $n_{D20.7} 1.4294$; hydrolysis of 20 g. VII by boiling 24 hrs. with alc.-aqueous NaOH , gives 19.8 g. 3,3,5-trimethyl-1-hexanecarboxylic acid, $b_8 132-3^\circ$, $n_{D21} 1.4346$; S-benzylthiuronium salt, m. 153° ; chloride (VIIA), $b_{22} 104^\circ$, $n_{D21} 1.4411$; amide, m. 107° ; Et ester (VIII), $b_9 96.5^\circ$, $n_{D21.2} 1.4254$. VIII (40 g.) in 60 ml. ether, added dropwise to III from 80.5 g. II in 150 ml. ether and refluxed 1 hr., gives 60 g. 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)-7-tridecanol (IX), $b_{0.8} 176-8^\circ$, $n_{D20} 1.4558$; dehydrogenation of 40 g. IX with iodine (3 hrs. at 200°) gives 31 g. 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)-7-tridecene (X), $b_{0.8} 161-2^\circ$, $n_{D26.4} 1.4548$; the action of O_3 on 8.6 g. X yields 1.9 g. 2,2,4,10,12,12-hexamethyl-7-tridecanone (XI), $b_{1.1} 124^\circ$, $n_{D20} 1.4460$ (semicarbazone, m. 69° ; 2,4-dinitrophenylhydrazone, m. 39°), and 2.8 g. VI. Hydrogenation of X in EtOH over Raney Ni ($180^\circ/27$ atmospheric) gives 78% 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)tridecane, $b_{0.5} 166^\circ$, $n_{D20} 1.4558$, $d_{2020} 0.8152$. VIIA

(from 20.5 g. acid) and (Me₃CCH₂CHMeCH₂)₂Cd (from 31 g. II) in C₆H₆ give 68% XI. III (from 32.5 g. II) and 37.6 g. AgBr, refluxed 1 hr., give 8.2 g. 2,2,4,9,11,11-hexamethyldodecane, b₁₀ 138.5°, n_{D20} 1.4370; much olefin is formed.

IT 2570-95-8, Heptanenitrile, 4,6,6-trimethyl-
(preparation of)

RN 2570-95-8 CAPLUS

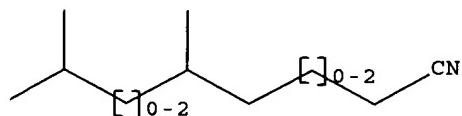
CN Heptanenitrile, 4,6,6-trimethyl- (7CI, 9CI) (CA INDEX NAME)



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L5 HAS NO ANSWERS

L5 STR



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L12 20 S L11

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

99.70

321.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-14.60

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